Sarcosylsarcosine, n-propoxycarbonyl-, undecyl ester

Inchi: InChI=1S/C21H40N2O5/c1-5-7-8-9-10-11-12-13-14-16-27-20(25)18-22(3)19(24)17-23(4)21(26)28-15-6-2

InchiKey: MTOOOSVVGZHZMD-UHFFFAOYSA-N

Formula: C21H40N2O5

SMILES: CCCCCCCCCCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCCC

Mol. weight [g/mol]: 400.55

Physical Properties

Property code	Value	Unit	Source
gf	-249.26	kJ/mol	Joback Method
hf	-943.89	kJ/mol	Joback Method
hfus	63.36	kJ/mol	Joback Method
hvap	91.48	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.997		Crippen Method
mcvol	343.160	ml/mol	McGowan Method
pc	1052.09	kPa	Joback Method
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook
tb	911.21	K	Joback Method
tc	1116.12	K	Joback Method
tf	585.62	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1139.87	J/mol×K	911.21	Joback Method
cpg	1157.45	J/mol×K	945.36	Joback Method
cpg	1173.71	J/mol×K	979.51	Joback Method
cpg	1188.70	J/mol×K	1013.66	Joback Method
cpg	1202.46	J/mol×K	1047.82	Joback Method
cpg	1215.03	J/mol×K	1081.97	Joback Method
cpg	1226.45	J/mol×K	1116.12	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320644&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume